

Benzamide, N,N,3-trimethyl-

Other names:	3-CH3-C6H4CON(CH3)2
Inchi:	InChI=1S/C10H13NO/c1-8-5-4-6-9(7-8)10(12)11(2)3/h4-7H,1-3H3
InchiKey:	SWYVHBPXKKDGLL-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	<chem>Cc1cccc(C(=O)N(C)C)c1</chem>
Mol. weight [g/mol]:	163.22
CAS:	6935-65-5

Physical Properties

Property code	Value	Unit	Source
affp	927.00	kJ/mol	NIST Webbook
basg	896.00	kJ/mol	NIST Webbook
gf	117.96	kJ/mol	Joback Method
hf	-69.72	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.697		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	526.17	K	Joback Method
tc	739.11	K	Joback Method
tf	323.80	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.47	J/molxK	703.62	Joback Method
cpg	310.22	J/molxK	526.17	Joback Method
cpg	324.55	J/molxK	561.66	Joback Method
cpg	338.00	J/molxK	597.15	Joback Method
cpg	350.61	J/molxK	632.64	Joback Method
cpg	362.42	J/molxK	668.13	Joback Method

cpg	383.78	J/mol×K	739.11	Joback Method
hvapt	29.90	kJ/mol	389.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	1.60	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6935655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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